



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 22, 2014 – 01:57 PM EDT

PDB ID : 4V99
Title : The Crystallographic Structure of Panicum Mosaic Virus
Authors : Makino, D.L.; Larson, S.B.; McPherson, A.
Deposited on : 2012-07-04
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : **NOT EXECUTED**
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : **NOT EXECUTED**
Percentile statistics : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.90 Å.

There are no percentiles available for this entry.

MolProbity and EDS were not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 588120 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Aa	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Ab	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ae	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Af	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Ag	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Aj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ak	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Al	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ao	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ap	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Aq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	At	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Au	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Av	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ay	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Az	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	A1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	A4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	A5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	A6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	BG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	BL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	BQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	BV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ba	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Be	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Bf	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Bj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Bk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Bo	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Bp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Bt	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Bu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	By	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Bz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	B1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	B4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	B5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	B6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	CB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	CG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	CQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	CV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ca	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ce	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Cf	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Cj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ck	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Co	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Cp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ct	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Cu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Cy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Cz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	C1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	C4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	C5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	C6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	DB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	DG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	DL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	DQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Da	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Db	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	De	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Df	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Dg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Dj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Dk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Di	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Do	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Dp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Dq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Dt	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Du	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Dv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Dy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Dz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	D1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	D4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	D6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	EC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	EH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	EM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	ER	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	EW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ea	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Eb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ee	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ef	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Eg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ej	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ek	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	El	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Eo	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ep	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Eq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Et	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Eu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Ev	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ey	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ez	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	E1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	E4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	E5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	E6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	FA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	FB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	FC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	FF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	FG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	FH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	FK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	FL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	FM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	FP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	FQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	FR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	FU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	FV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	FW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	FZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Fa	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Fb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Fe	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ff	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Fg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Fj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Fk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Fl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Fo	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Fp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Fq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ft	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Fu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Fv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Fy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Fz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	F1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	F4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	F5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	F6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	GA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	GB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	GC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	GF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	GG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	GH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	GK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	GL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	GM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	GP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	GQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	GR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	GU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	GV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	GW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	GZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ga	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ge	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Gf	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Gj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Gk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Go	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Gp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Gt	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Gu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Gy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Gz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	G1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	G4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	G5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	G6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ha	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	He	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hf	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Hj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ho	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ht	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Hy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	H1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	H4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	H5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	H6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	IB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	IG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	IL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	IQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	IV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ia	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Ib	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ie	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	If	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Ig	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ij	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ik	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Il	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Io	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ip	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Iq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	It	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Iu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Iv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Iy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Iz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	I1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	I4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	I5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	I6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	JA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	JB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	JC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	JF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	JG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	JH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	JK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	JL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	JM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	JP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	JQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	JR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	JU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	JV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	JW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	JZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ja	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Jb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Je	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Jf	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Jg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Jj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Jk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Jl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Jo	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Jp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Jq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Jt	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ju	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Jv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Jy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Jz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	J1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	J4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	J5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	J6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			

- Molecule 2 is a RNA chain called 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AD	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	AI	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	AN	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	AS	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	AX	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Ac	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Ah	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Am	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Ar	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Aw	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	A2	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Bc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Bh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Bm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Br	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Bw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	B2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	B7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Cc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Ch	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Cm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Cr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Cw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	C2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	C7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	D2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	D7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	ED	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	EI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	EN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	ES	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	EX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Ec	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Eh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Em	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Er	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Ew	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	E2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	E7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	FD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	FI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	FN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	FS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	FX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Fc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Fh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Fm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Fr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Fw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	F2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	F7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	GD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	GI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	GN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	GS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	GX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	G2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	G7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	H2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	ID	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	II	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	IN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	IS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	IX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Ic	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Ih	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Im	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Ir	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Iw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	I2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	I7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Jc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Jh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Jm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Jr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Jw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	J2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	J7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Jt	1	Total 1	Ca 1	0	0
3	FU	1	Total 1	Ca 1	0	0
3	CA	1	Total 1	Ca 1	0	0
3	IZ	1	Total 1	Ca 1	0	0
3	Eo	1	Total 1	Ca 1	0	0
3	FK	1	Total 1	Ca 1	0	0
3	DZ	1	Total 1	Ca 1	0	0
3	Ce	1	Total 1	Ca 1	0	0
3	Af	1	Total 1	Ca 1	0	0
3	EF	1	Total 1	Ca 1	0	0
3	JL	1	Total 1	Ca 1	0	0
3	C4	1	Total 1	Ca 1	0	0
3	Gt	1	Total 1	Ca 1	0	0
3	Df	1	Total 1	Ca 1	0	0
3	HF	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Be	1	Total 1	Ca 1	0	0
3	AA	1	Total 1	Ca 1	0	0
3	Hj	1	Total 1	Ca 1	0	0
3	JA	1	Total 1	Ca 1	0	0
3	A4	1	Total 1	Ca 1	0	0
3	D4	1	Total 1	Ca 1	0	0
3	AL	1	Total 1	Ca 1	0	0
3	JZ	1	Total 1	Ca 1	0	0
3	DP	1	Total 1	Ca 1	0	0
3	Hg	1	Total 1	Ca 1	0	0
3	GK	1	Total 1	Ca 1	0	0
3	HZ	1	Total 1	Ca 1	0	0
3	JF	1	Total 1	Ca 1	0	0
3	EU	1	Total 1	Ca 1	0	0
3	AF	1	Total 1	Ca 1	0	0
3	CZ	1	Total 1	Ca 1	0	0
3	Ek	1	Total 1	Ca 1	0	0
3	Bo	1	Total 1	Ca 1	0	0
3	DK	1	Total 1	Ca 1	0	0
3	DF	1	Total 1	Ca 1	0	0
3	GA	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	DU	1	Total 1	Ca 1	0	0
3	Ao	1	Total 1	Ca 1	0	0
3	Jy	1	Total 1	Ca 1	0	0
3	CU	1	Total 1	Ca 1	0	0
3	Co	1	Total 1	Ca 1	0	0
3	Gj	1	Total 1	Ca 1	0	0
3	Et	1	Total 1	Ca 1	0	0
3	Cy	1	Total 1	Ca 1	0	0
3	BU	1	Total 1	Ca 1	0	0
3	Aj	1	Total 1	Ca 1	0	0
3	HP	1	Total 1	Ca 1	0	0
3	FF	1	Total 1	Ca 1	0	0
3	CP	1	Total 1	Ca 1	0	0
3	DA	1	Total 1	Ca 1	0	0
3	AU	1	Total 1	Ca 1	0	0
3	Ht	1	Total 1	Ca 1	0	0
3	GZ	1	Total 1	Ca 1	0	0
3	EK	1	Total 1	Ca 1	0	0
3	Fo	1	Total 1	Ca 1	0	0
3	Ct	1	Total 1	Ca 1	0	0
3	BZ	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	FP	1	Total 1	Ca 1	0	0
3	Bk	1	Total 1	Ca 1	0	0
3	GP	1	Total 1	Ca 1	0	0
3	AP	1	Total 1	Ca 1	0	0
3	I1	1	Total 1	Ca 1	0	0
3	Ft	1	Total 1	Ca 1	0	0
3	At	1	Total 1	Ca 1	0	0
3	B5	1	Total 1	Ca 1	0	0
3	IR	1	Total 1	Ca 1	0	0
3	BF	1	Total 1	Ca 1	0	0
3	BQ	1	Total 1	Ca 1	0	0
3	I4	1	Total 1	Ca 1	0	0
3	CG	1	Total 1	Ca 1	0	0
3	HK	1	Total 1	Ca 1	0	0
3	G1	1	Total 1	Ca 1	0	0
3	A1	1	Total 1	Ca 1	0	0
3	FZ	1	Total 1	Ca 1	0	0
3	AZ	1	Total 1	Ca 1	0	0
3	Ho	1	Total 1	Ca 1	0	0
3	BK	1	Total 1	Ca 1	0	0
3	If	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G4	1	Total 1	Ca 1	0	0
3	J4	1	Total 1	Ca 1	0	0
3	Jj	1	Total 1	Ca 1	0	0
3	Ey	1	Total 1	Ca 1	0	0
3	Je	1	Total 1	Ca 1	0	0
3	IA	1	Total 1	Ca 1	0	0
3	JP	1	Total 1	Ca 1	0	0
3	GF	1	Total 1	Ca 1	0	0
3	Dj	1	Total 1	Ca 1	0	0
3	EP	1	Total 1	Ca 1	0	0
3	Dy	1	Total 1	Ca 1	0	0
3	HA	1	Total 1	Ca 1	0	0
3	Dt	1	Total 1	Ca 1	0	0
3	H4	1	Total 1	Ca 1	0	0
3	Jo	1	Total 1	Ca 1	0	0
3	Go	1	Total 1	Ca 1	0	0
3	IK	1	Total 1	Ca 1	0	0
3	BB	1	Total 1	Ca 1	0	0
3	JU	1	Total 1	Ca 1	0	0
3	EZ	1	Total 1	Ca 1	0	0
3	Do	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Io	1	Total 1	Ca 1	0	0
3	Fk	1	Total 1	Ca 1	0	0
3	CK	1	Total 1	Ca 1	0	0
3	Ge	1	Total 1	Ca 1	0	0
3	IU	1	Total 1	Ca 1	0	0
3	FA	1	Total 1	Ca 1	0	0
3	Bt	1	Total 1	Ca 1	0	0
3	IF	1	Total 1	Ca 1	0	0
3	F4	1	Total 1	Ca 1	0	0
3	Fe	1	Total 1	Ca 1	0	0
3	HU	1	Total 1	Ca 1	0	0
3	Ij	1	Total 1	Ca 1	0	0
3	Cj	1	Total 1	Ca 1	0	0
3	Hy	1	Total 1	Ca 1	0	0
3	Ee	1	Total 1	Ca 1	0	0
3	By	1	Total 1	Ca 1	0	0
3	GU	1	Total 1	Ca 1	0	0
3	F1	1	Total 1	Ca 1	0	0
3	E4	1	Total 1	Ca 1	0	0
3	EC	1	Total 1	Ca 1	0	0
3	It	1	Total 1	Ca 1	0	0

3 Residue-property plots

MolProbity and EDS were not executed - this section will therefore be empty.

4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	411.74Å 403.90Å 412.46Å 90.00° 89.65° 90.00°	Depositor
Resolution (Å)	50.01 – 2.90	Depositor
% Data completeness (in resolution range)	74.9 (50.01-2.90)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.91Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.251 , 0.285	Depositor
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.138	Xtriage
Estimated twinning fraction	0.025 for -l,k,h 0.034 for -h,-l,-k 0.024 for -h,l,k 0.044 for -k,-h,-l 0.024 for k,h,-l 0.017 for -l,-h,k 0.030 for -k,l,-h 0.038 for l,h,k 0.027 for k,-l,-h 0.035 for h,-k,-l 0.030 for -l,-k,-h	Xtriage
L-test for twinning	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 2217465 reflections	Xtriage
Total number of atoms	588120	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

MolProbity was not executed - this section will therefore be empty.

5.2 Close contacts ⓘ

MolProbity was not executed - this section will therefore be empty.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

MolProbity was not executed - this section will therefore be empty.

5.3.2 Protein sidechains ⓘ

MolProbity was not executed - this section will therefore be empty.

5.3.3 RNA ⓘ

MolProbity was not executed - this section will therefore be empty.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

validation-pack was not executed - this section will therefore be empty.

5.5 Carbohydrates ⓘ

validation-pack was not executed - this section will therefore be empty.

5.6 Ligand geometry ⓘ

validation-pack was not executed - this section will therefore be empty.

5.7 Other polymers ⓘ

validation-pack was not executed - this section will therefore be empty.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.